Nomenclature of Polymers

by

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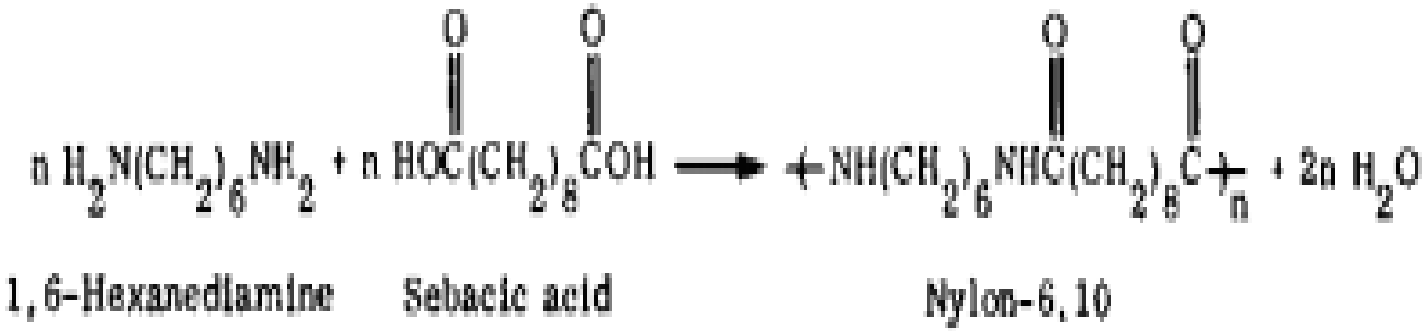
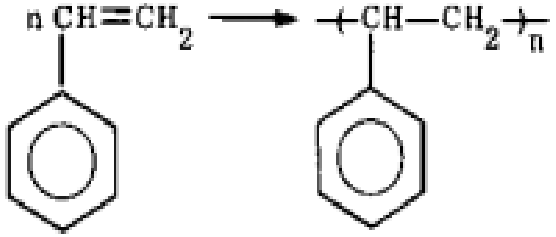
COMMON NAMES

Some polymers are named as per their place of origin, such as *Hevea brasiliensis*- i.e **“rubber from Brazil”-**for natural rubber. Some are named after their discoverer, as is Bakelite, condensation polymer of phenol and formaldehyde, which was commercialized by Leo Baekeland in 1905. The nylons were named according to the number of carbons in the diamine and carboxylic acid reactants (monomers) used in their syntheses. The nylon produced by the condensation of 1,6-hexanediamine (6 carbons) and sebacic acid (10 carbons) is called nylon-6,10. Similarly, the polymer from 1,6-hexanediamine and adipic acid (each with 6 carbons) is called nylon-6,6 or nylon-66, and the nylon from the single reactant caprolactam (6 carbons) is called nylon-6.



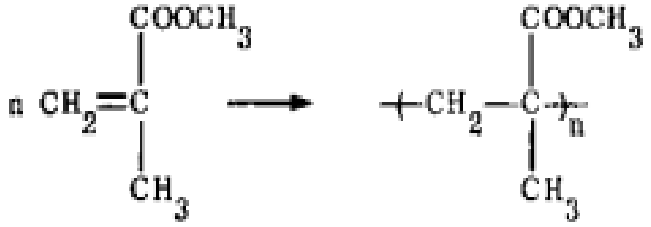
SOURCE-BASED NAMES

Most polymer names used by polymer scientists are source-based; i.e., they are based on the common name of the reactant monomer, preceded by the prefix "poly." For example, polystyrene is the most frequently used name for the polymer derived from the monomer 1-phenylethene, which has the common name styrene.



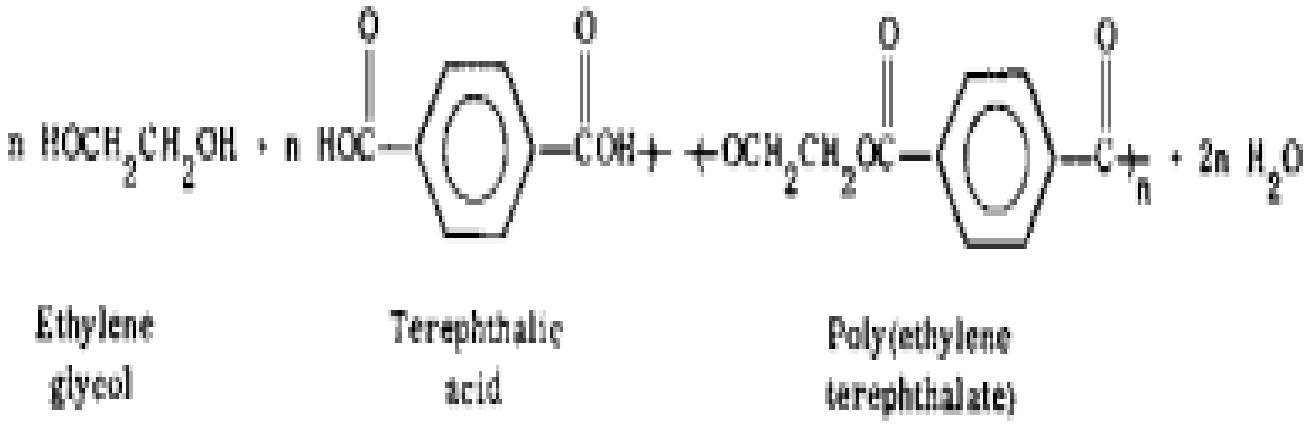
Styrene Polystyrene

The vast majority of polymers based on the vinyl group (CH2=CHX) or the vinylidene group (CH2=CX2) as the repeat unit are known by their source-based names. For example, polyethylene is derived from the monomer ethylene, poly (vinyl chloride) from the monomer vinyl chloride, and poly (methyl methacrylate) from methyl methacrylate



Methyl methacrylate Poly(methyl methacrylate)

In the case of poly(ethylene terephthalate), the glycol portion of the name of the monomer, ethylene glycol, is used in constructing the polymer name, so that the name is actually a hybrid of a source based and a structure-based name.



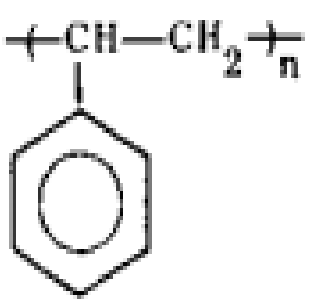
This polymer is well known by trade names, such as Dacron, or its common grouping, polyester. Thus there exists a variety of practices with respect to even source based names.

Copolymers are composed of two or more monomer units. Source-based names are conveniently used to describe copolymers by using an appropriate term between the names of the monomers. Different connecting terms may be used, depending on what is known about the structure of the copolymer. When no information is specified about the sequence of monomer units in the copolymer, the connective term *co* is used in the general format poly(A-*co*-B), where A and B are the names of the two monomers. An unspecified copolymer of styrene and methyl methacrylate would be called poly [styrene-*co*-(methyl methacrylate)]. Kraton, the yellow rubber-like material found on the bottom of many running shoes, is formed from a group of styrene units, i.e., a "block" of polystyrene, attached to a group of butadiene units, or a block of polybutadiene, which is attached to another block of polystyrene forming a triblock copolymer. The general representation of such a block copolymer is −AAABBBAAA−, where each A or B represents an individual monomer unit. The proper source-based name for Kraton is polystyrene-*block*-polybutadiene *bloc k*polystyrene, with the prefix "poly" being retained for each block.

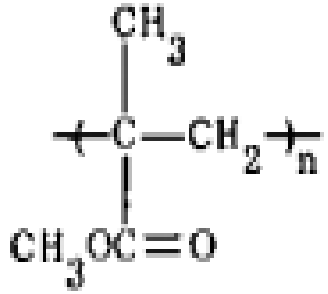
STRUCTURE-BASED NAMES

Although source-based names are generally employed for simple polymers, IUPAC, has framed systems for the naming of more complex polymers. The IUPAC system names the components of the repeat unit, arranged in a prescribed order. The rules for selecting the order of the components to be used as the repeat unit are found elsewhere. However, once the order is selected, the naming can be made as follows.

Polystyrene



Poly(1-phenylethylene)

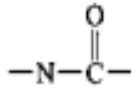
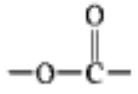
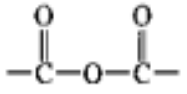
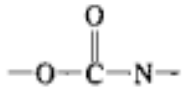
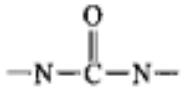
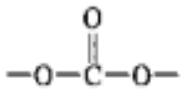
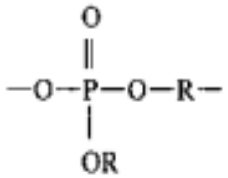


Poly[1-(methoxycarbonyl)-1-methylethylene]

Source-based names	Structure-based names
Polyacrylonitrile	Poly(1-cyanoethylene)
Poly(ethylene oxide)	Polyoxyethylene
Poly(ethylene terephthalate)	Polyoxyethyleneoxyterephthaloyl
Polyisobutylene	Poly(1,1-dimethylethylene)
Poly(methyl methacrylate)	Poly[(1-methoxycarbonyl)-1-methylethylene]
Polypropylene	Poly(1-methylethylene)
Polystyrene	Poly(1-phenylethylene)
Polytetrafluoroethylene	Polydifluoromethylene
Poly(vinyl acetate)	Poly(1-acetoxyethylene)
Poly(vinyl alcohol)	Poly(1-hydroxyethylene)
Poly(vinyl chloride)	Poly(1-chloroethylene)
Poly(vinyl butyral)	Poly[(2-propyl-1,3-dioxane-4,6-diyl)methylene]

LINKAGE-BASED NAMES

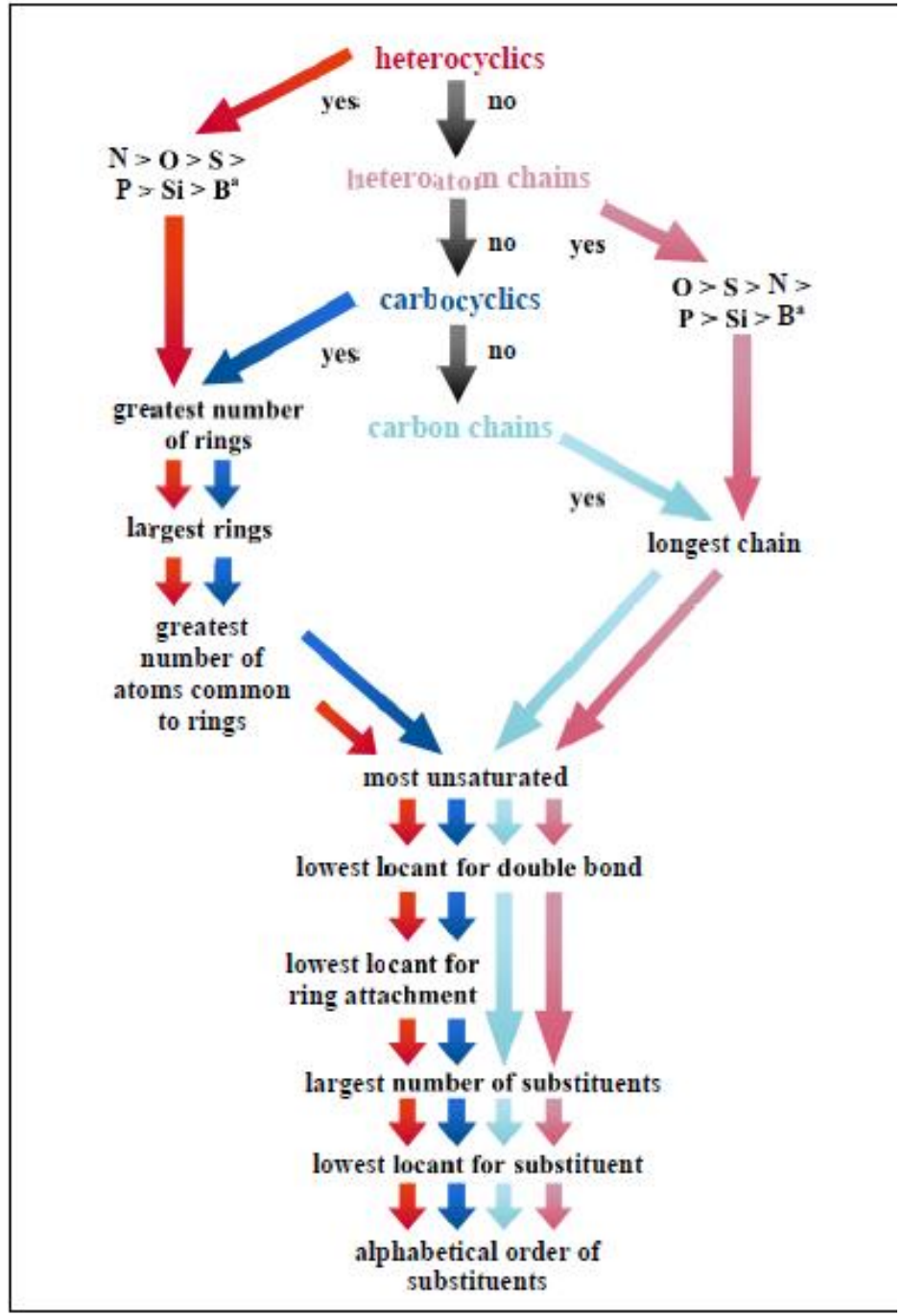
Many polymer "families" are referred to by the name of the particular linkage that connects the polymers .The family name is "poly" followed by the linkage name. Thus, polymers containing the carbonate linkage are known as polycarbonates; those containing the ether linkage are called polyethers, etc.

Family name	Linkage	Family name	Linkage
Polyamide		Polyvinyl	
Polyester		Polyanhydride	
Polyurethane		Polyurea	
Polyether		Polycarbonate	
		Polyphosphate ester	
Polysiloxane			
Polysulfide		Polysulfones	

GENERAL RULES

In the chemical literature in particular, systems based on Chemical Abstracts—searches for particular polymers can be conducted using the Chemical Abstracts Service number, (CAS) (where known) or the repeat unit. The International Union of Pure and Applied Chemistry (IUPAC) and CAS have agreed on a set of guidelines for the identification, orientation, and naming of polymers based on the structural repeat unit (SRU). IUPAC refers to polymers as "poly(constitutional repeating unit)" but CAS utilizes a "poly(structural repeating unit)." These two approaches typically give similar results. Here we will practice using the sequence ***"Identification ---- Orientation ----- Naming,"*** first by giving some general principles and finally by using specific examples.

In the *identification* step, the structure is drawn, usually employing at least two repeat units. Next, in the *orientation* step, the guidelines are applied. Here we concentrate on basic guidelines. Within these guidelines are subsets of guidelines that are beyond the scope of this class. Structures will generally be drawn in the order, from left to right, in which they are to be named.

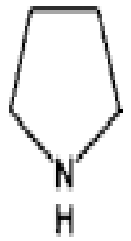

heterocyclics
yes
no
N > O > S > P > Si > B[a]
heteroatom chains
no
yes
O > S > N > P > Si > B[a]
carbocyclics
yes
no
greatest number of rings
carbon chains
largest rings
yes
longest chain
greatest number of atoms common to rings
most unsaturated
lowest locant for double bond
lowest locant for ring attachment
largest number of substituents
lowest locant for substituent
alphabetical order of substituents

SENIORITY

The starting point for the naming of a polymer unit involves determining seniority among the subunits.

A. This order is Heterocyclic rings> Greatest number of most preferred acyclic heteroatoms > Carbocyclic rings > Greatest number of multiple bonds > Shortest path or route (or lowest locant) to these substituents > Chains containing only carbon atoms.

Heterocyclic ring > Acyclic hetero atoms > Carbocyclic rings



> —O—CH_2— >

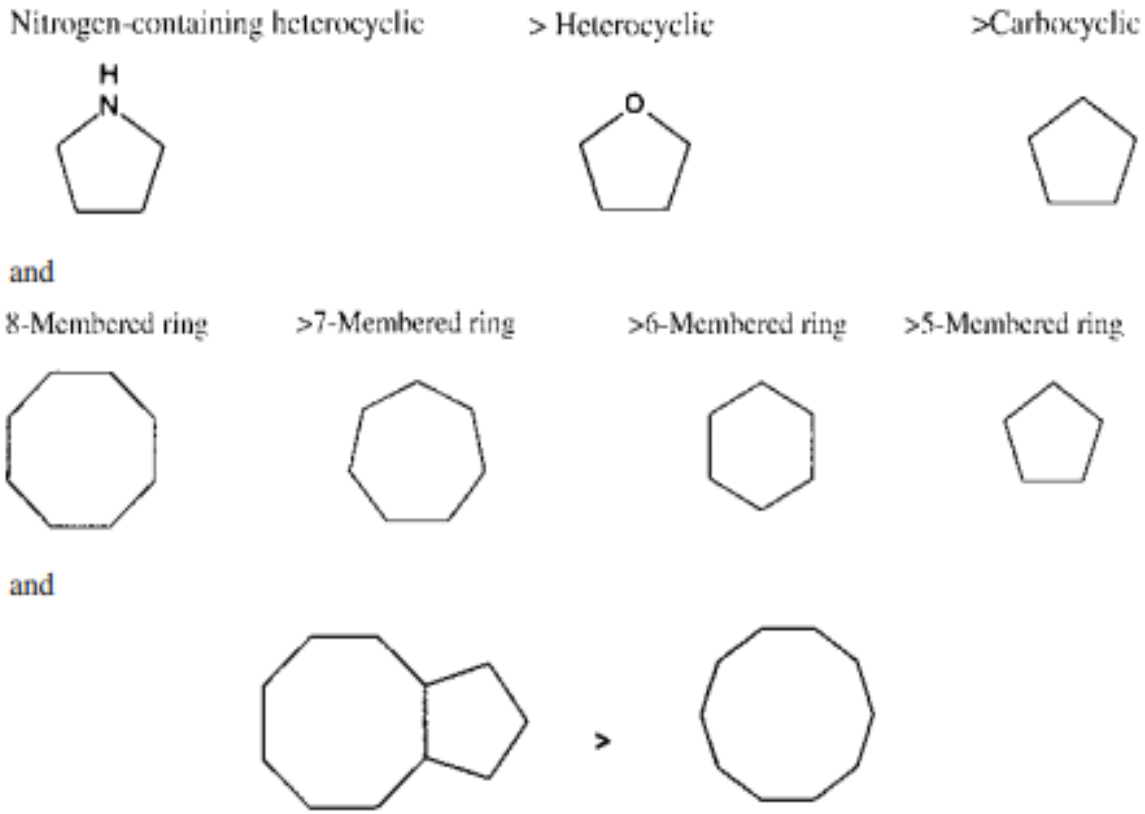
> Multiple bonds > Lowest locant > Only carbon chains

> —CH=CH— > —CF_2—CHF > —CHF—CF_2— > —CH_2—CH_2—

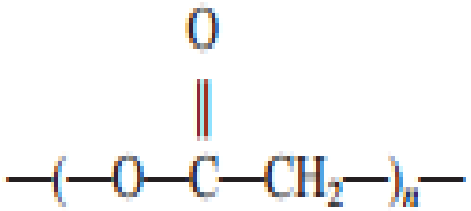
The lowest locant or shortest distance refers to the number of atoms from one senior subunit to the next most senior subunit when there is only one occurrence of the senior subunit. ***This order refers to the backbone and not substitutions.*** Thus, polystyrene and poly(vinyl chloride) are contained within the "chains containing only carbon atoms" grouping.

B. For ring systems the overall seniority is Heterocyclic > Carbocyclic,

But within the rings there seniority is in the order; Nitrogenous heterocyclic > Heterocyclic > Largest number of rings > Cyclic system occurring earliest in the following list of systems spiro, bridged fused, bridges nonfused, fused > Largest individual ring (applies to fused carbocyclic systems) Greatest number of ring atoms For example,



C. For linear chains or cyclic rings containing hetero-atoms, the order is (decreasing order) O S Se Te N P As Sb Bi Si Ge Sn Pb B Hg. Thus, because –O–CH2–is senior to –S–CH2–, it would be named first in a polymer that contained both –O–CH2– and –S–CH2– segments. Further, a polymer containing these alternating units would *not* be ~~poly(thiomethyleneoxymethylene)~~ but would be named poly(oxymethylenethiomethylene).



is named poly[oxy(1-oxy-1,2-ethanediyl)] or less preferred poly[oxy(1-oxoethylene)] but not ~~poly[(2-oxo-1,2-ethanediyl)oxy] or poly[(2-oxoethylene)oxy].~~

D. In rings, unsaturation is senior to saturation. The more unsaturated, the more senior with all other items being equal. Thus 1,4-phenylene is senior to 2,5-cyclohexadiene-1,4-diyl, which in turn is senior to 2-cyclohexene-1,4-diyl, which is senior to 1,4-cyclohexaned iyl. For linear chains –CH=CH-CH=CH– > –CH=CH–CH2–CH2– > the totally saturated chain segment.

ROUTE

A. From the senior subunit determined from "Seniority" take the shortest path (smallest number of atoms) to another like or identical unit or to the next most preferred subunit. Thus for the homopolymer poly(oxymethylene) it is simply going from one oxygen to the next oxygen and recognizing that this is the repeat unit. For a more complex ether this means going until the chain begins to repeat itself going in the shortest direction from the senior unit or atom to the next most senior unit or atom. Thus, –O–C–C–O–C–C–C– is named "oxy-1,2-ethanediyloxy-1,3-propanediyl" rather than ~~"oxy- 1,3-propanediyloxy-1,2-ethanediyl.~~

B. Where path lengths are equal, e.g nylons, the repeat unit is named so that the heteroatom "N" is first named prior to more highly substituted (carbonyl) unit. Thus, nylon 3,3, with the structure is named poly [imino(1,3-dioxo-1,3-propanediyl)imino-1,3-propanediyl].

C. In otherwise identical subunits, there are three items to be considered in decreasing order of importance:

1.Maximum substitution: thus, 2,3,5-trichloro-*p*-phenylene > 2,5-dichloro-*p* phenylene > 2-chloro-*p*-phenylene,

2. Lowest locants: thus, 2,3-dichloro-*p*-phenylene > 2,5-dichloro-*p*-phenylene

3. Earliest alphabetical order: thus, 2-bromo-*p*-phenylene > 2-chloro-*p*phenylene > *2*-iodo-*p*-phenylene.

D. Where there is no conflict with other guidelines, multiple bonds should be assigned the lowest locants; in rings, double bonds > single bonds; in acyclic carbon chains, double bonds > triple bonds, > single bonds. Thus, the polymer from 1,3-butanediene polymerized in the so-called "1,4–" mode is usually drawn as –(–C–C=C–C–)– but it is named as drawn as –(–C=C–C–C–)– and named poly(1-butene-1,4-diyl) with the appropriate "cis-" or "trans-" designation.

Polyisoprene, typically drawn as is frequently named poly(2-methyl-1,3-butadiene) but it is named as though its structure is with the name poly(1-methyl-1-butene-1,4-diyl). Substituents are named as one of several classes. The most important ones are dealt with here. For monoatomic radicals from borane, methane, silane (and other Group IVA elements) they are named by replacing the "ane" ending with "yl," "ylene," and "ylidyne" to denote the loss of one, two, or three hydrogen atoms, respectively.

H_2B— boryl H_3C— methyl H_2C= methylene HC≡ methylidyne

Acyclic hydrocarbon radicals are named from the skeletons by replacing "ane," "ene," and "yne" suffixes by "yl," "enyl," and "ynyl," respectively.

CH_3—CH_2— ethyl CH_3—CH_2—CH_2— propyl —CH_2—CH_2— 1,2-ethanediyl

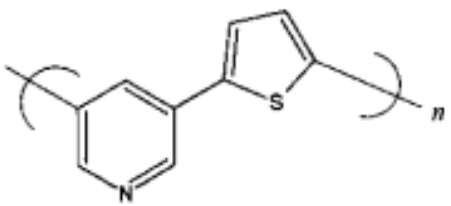
—CH=CH— 1,2-ethenediyl H_2C=CH—CH=2-propenylidene

—CH_2—C(=)—CH_2— 1,3-propanediyl-2-ylidene

—CH_2—CH(|)—CH_2— 1,2,3-propanetriyl

Examples

Following are examples that illustrate CAS guidelines for naming.

—$(CH_2—)_n$—	Poly(methylene) (to locate poly(methylene) in the Registry file by name, search for "Ethane, homopolymer")
—$(CH_2—CH_2—)_n$—	Poly(ethylene) (to search for poly(ethylene) search for "Ethane, homopolymer")
—$(CH{=}CH—)_n$—	Poly(1,2-ethenediyl)
—$(C(=O)—C(=O)—CH_2—CH_2—)_n$—	Poly1,2-dioxo-1,4-butanediyl
—$(—CH{=}CH—CH(CH_3)—CH_2—)_n$—	Poly(3-methyl-1-butene-1,4-diyl
—$(NH—C(=O)—CH_2—CH_2—)_n$—	Poly[imino(1-oxo-1,3-propanediyl)]
—$(—O—C(=O)—O—CH_2CH_2—)_n$—	Poly[oxocarbonyloxy(1,2-ethanediyl)]
—$(—O—CH_2—S—CH_2—NH—CH_2—CH_2—S—NH-CH_2—CH_2—)_n$—	Poly(oxymethylenethiomethyleneimino-1,2-ethanediylthioimino-1,2-ethanediyl)
—$(—CFH—CH_2—)_n$—	Poly(1-fluoro-1,2ethanediyl) search for under "Ethene, fluoro-homopolymer")
—$(—O—CH_2—CH_2—)_n$—	Poly(oxy-1,2-ethanediyl)
—$(—O—CH_2—)_n$—	Poly(oxymethylene)
	Poly(3,5-pyridinediyl-2,5-thiophenediyl)
—$[—NH—C(=O)—(CH_2)_4—C(=O)—NH—(CH_2)_6—]_n$—	Poly[imino(1,6-dioxo-1,6hexanediyl)imino-1,6-hexanediyl]

Acknowledgement

1.Polymer Chemistry, Charles E Carraher, Jr, sixth edition

2. A Brief Guide to Polymer Nomenclature ; International Union of Pure and Applied Chemistry; Subcommittee on Polymer Terminology;Version 1.1 (2012)